Finite-temperature Drude weight within the anisotropic Heisenberg chain

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Finite-temperature Drude weight (spin stiffness) $D(T)$ is evaluated within the anisotropic spin-$1/2$ Heisenberg model on a chain using the exact diagonalization for small systems. It is shown that odd-side chains allow for more reliable scaling and results, in particular if one takes into account corrections due to low-frequency finite-size anomalies. At high T and zero magnetization D is shown to scale to zero approaching the isotropic point $\Delta = 1$. On the other hand, for $\Delta > 2$ at all magnetizations D is nearly exhausted with the overlap with the conserved energy current. Results for the T-variation $D(T)$ are also presented.

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I. INTRODUCTION

It has by now become evident that many-body (MB) quantum systems of interacting particles behave with respect to transport quite differently if they are either integrable or non-integrable [1, 2]. In integrable systems the anomalous response shows up in a possibility of finite-temperature stiffness (Drude weight) $D(T) > 0$ [3], both the charge (or spin) and the thermal one [5], indicating the dissipationless d.c. transport at $T > 0$. The prototype model for this phenomenon is the anisotropic spin-$1/2$ Heisenberg model on a chain, equivalent to the one-dimensional (1D) t-V model of spinless fermions with nearest neighbor repulsion. Within this model one of the conserved quantities is the energy current j_E leading to the singular but trivial thermal dynamical-conductivity linear response [5], i.e., $\kappa(\omega) = D_T\delta(\omega)$. On the other hand, the spin current j and the corresponding dynamical spin conductivity (diffusivity) $\sigma(\omega)$ at $T > 0$ is still the subject of very active theoretical investigations and debate.

In the case of a nonvanishing projection of the spin current j on local conserved quantities Q_n the Mazur inequality offers a firm proof of finite $D(T \neq 0) > 0$ [5] in the thermodynamic limit . Still, at zero magnetization, i.e., at the total spin $S^z = 0$ the overlap with all Q_n vanishes independent of the anisotropy Δ [5]. To employ the same argument one possible path is to construct more general nonlocal conserved quantities [6, 7] which should be further explored.

The (original) alternative formulation via the MB level dynamics induced in a 1D ring via an external flux [3, 4] offers a qualitative understanding and is the starting point for numerical calculations using the full exact diagonalization (ED) method [8–11]. The latter so far did not eliminate disagreement on several questions : a) is D a monotonous function of Δ at fixed S^z [10], b) does $D(T > 0)$ vanish on approaching the isotropic point $\Delta = 1, S^z = 0$ [9, 12], c) which if any analytical result, obtained via the Thermodynamic Bethe Ansatz [13, 15], is correct and compatible with numerical investigations.

In the following we present results of the numerical study for $D(T)$ as obtained using the ED and the scaling for small systems. In contrast to previous works [9, 10] we perform the study within the canonical ensemble which offers much faster convergence with the chain size L, at least approaching the isotropic point $\Delta \sim 1, S^z \sim 0$. To avoid quite singular behavior of even-lengths chains, we study spin systems with odd L. In particular, we pay the attention to possible low-frequency contributions in the dynamical conductivity $\sigma(\omega)$ which can give an insight into anomalies around commensurate $\Delta = \cos(\pi/\nu)$ with integer ν, e.g., at $\Delta < 0.5$.

The paper is organized as follows: In Sec. II we present the model and Drude weight D as zero frequency contribution to dynamical conductivity. We shortly also describe numerical method used to analyse it. Our results are presented in Sec. III. First we investigate the high-temperature limit $C = TD$, where we emphasize the low-frequency contributions which can mask the correct result. We show also that within Ising-type regime $\Delta > 1$ the Drude weight calculated via the overlap with the conserved energy current gives nearly perfect results. Finally we focus on the temperature variation of $D(T)$.

II. DRUDE WEIGHT

We study the anisotropic $S = 1/2$ Heisenberg model on a chain with L sites and periodic boundary conditions

$$H = J\sum_{i=1}^{L}(S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + \Delta S^z_i S^z_{i+1}), \qquad (1)$$

where S^α_i are component of the $S = 1/2$ spin operators. In order to define the Drude weight (spin stiffness) D it is convenient to map the model (1) via the Jordan-Wigner transformation onto the t-V model of interacting spinless fermions adding a fictitious magnetic flux $\Phi = L\phi$ through the ring [4, 14], entering the hopping matrix elements,

$$H = t\sum_i (e^{i\phi}c^\dagger_i c_{i+1} + \text{h.c.}) + V\sum_i \Big(n_i - \frac{1}{2}\Big)\Big(n_{i+1} - \frac{1}{2}\Big), \qquad (2)$$

$n_i = c^\dagger_i c_i$, $t = J/2$ and $V = 2t\Delta$. Here we consider only chains with odd number of fermions N to avoid additional

boundary fermionic sign and other finite-size effects discussed in more detail below. In the following we use everywhere $J = 1$ in order to facilitate the comparison with the majority of previous works and references [9, 10, 13]. Note that relevant parameters are now the total spin S_z and magnetization $s = S_z/L$ or the fermion density or band filling $n = N/L = s + 1/2$.

Via the corresponding spin (particle or charge within the fermionic model) current

$$j = t\sum_i (ie^{i\phi}c_i^\dagger c_{i+1} + \text{h.c.}), \quad (3)$$

one can express the dynamical (spin) conductivity at general temperature $T > 0$ as

$$\sigma(\omega) = 2\pi D\delta(\omega) + \sigma_{reg}(\omega), \quad (4)$$

where the regular part $\sigma_{reg}(\omega)$ expressed in terms of eigenstates $|n\rangle$ and eigenenergies ϵ_n,

$$\sigma_{reg}(\omega) = \frac{\pi}{L}\frac{1-e^{-\beta\omega}}{\omega}\sum_{\epsilon_n\neq\epsilon_m} p_n|\langle n|j|m\rangle|^2\delta(\epsilon_n-\epsilon_m-\omega), \quad (5)$$

while the dissipationless component with the Drude weight (spin stiffness) D can be related to the flux dependence of MB states [3], in analogy with the original formulation by Kohn [14]

$$D = \frac{1}{2L}\sum_n p_n \frac{\partial^2\epsilon_n(\phi)}{\partial\phi^2}, \quad (6)$$

where $p_n = \exp(-\beta\epsilon)/Z$ are corresponding Boltzmann factors.

The relation (6) is convenient for the ED numerical evaluation of $D(T)$ in small systems, since it only requires the calculation of eigenvalues $\epsilon_n(\phi)$. Finally we are interested in the result within the thermodynamic limit $L \to \infty$ at fixed T and magnetization s (filling n) , hence several strategies to obtain the thermodynamic value are possible. Since we mostly consider the high-T limit (allowing for most accurate ED results in small systems) and ED sizes are quite limited $L \leq 21$, we perform the canonical calculation at total spin S^z (fermion number N). The grand canonical evaluation at available L and high T has a very broad distribution of N, leading to overestimates of D (or at least its slow convergence with L) in the vicinity of the isotropic phase, i.e., at $s \sim 0, \Delta \sim 1$. On the other hand, also results with even L show deficiencies [10]. Treating in Eq.(6) the flux ϕ as parameter, corresponding $D(\phi, T \gg 0)$ show strong anomaly at $\phi \to 0$ for even L and even N due to the particle-hole symmetry and degeneracy of MB levels. In addition, even-L systems give at odd N considerably lower values for D at $\Delta < 1$ and small L [10] (an origin could be also particle-hole symmetry absent at odd L) remedied presumably only at much larger L. To avoid these complications, we in the following consider only systems with odd $L = 5-21$ (for $L = 21$ only one k-vector due to very high CPU requirements) which reveal much weaker and more regular $D(\phi)$ dependence.

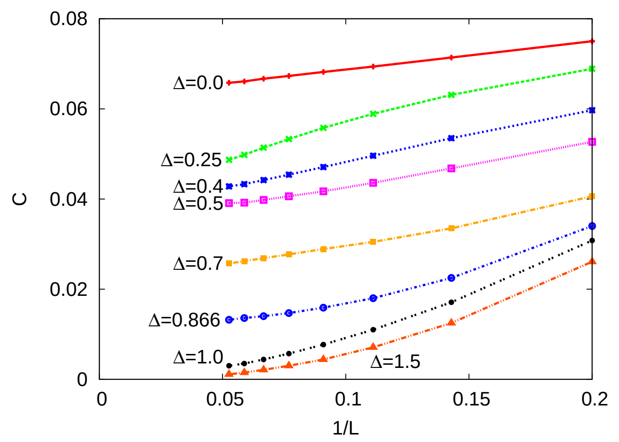

Figure 1. (Color online) High-T Drude weight $C = TD$ vs. $1/L$ for zero magnetization $s = 0$ and different Δ as obtained for systems with odd $L = 5-19$.

III. RESULTS

A. High-Temperature Limit.

In the following we mostly concentrate on the limit $T \to \infty$, expecting that obtained results are quite generic and qualitatively similar at any $T > 0$. Since for $T \to \infty$, $D(T)$ scales as $1/T$ the relevant and nontrivial quantity is $C = TD(T)$, representing also the limiting value of the current-current correlation function $C = C_{jj}(t \to \infty)$ [5]. Let us first consider the most delicate zero-magnetization $s = 0$ (half-filling $n = 1/2$) case. Since we choose odd L, the actual calculations are performed for closest odd $N = (L \pm 1)/2$. Results for C vs. $1/L$ for all odd $L = 5-19$ are presented for different Δ in Fig. 1. Several conclusions can be drawn directly from obtained results: a) Both values as well as the scaling with L are qualitatively different between $\Delta \geq 1$ and $\Delta < 1$. It is evident that for $\Delta \geq 1$ the only consistent limit appears to be $C = 0$. b) There are some visible anomalies near $\Delta < 0.5$ which indicate on a nonuniform dependence of $C(\Delta)$ [10] and in particular different scaling $L \to \infty$ which we discuss in more detail below.

In order to resolve the origin of the deviations of C at $\Delta < 0.5$ as well as of quite regular convergence of results for other values of Δ we investigate the dynamical $\sigma(\omega)$, shown conveniently also in the integrated form for $T \to \infty$,

$$I(\omega) = C + \frac{T}{\pi}\int_0^\omega \sigma_{reg}(\omega')d\omega', \quad (7)$$

consistent with the sum rule

$$I(\omega \to \infty) = Te_{kin} = -T\langle H_{kin}\rangle/L, \quad (8)$$

where H_{kin} is the kinetic-energy part in the model (2). e_{kin} can be evaluated exactly in the $\beta \to 0$ limit, even for finite L

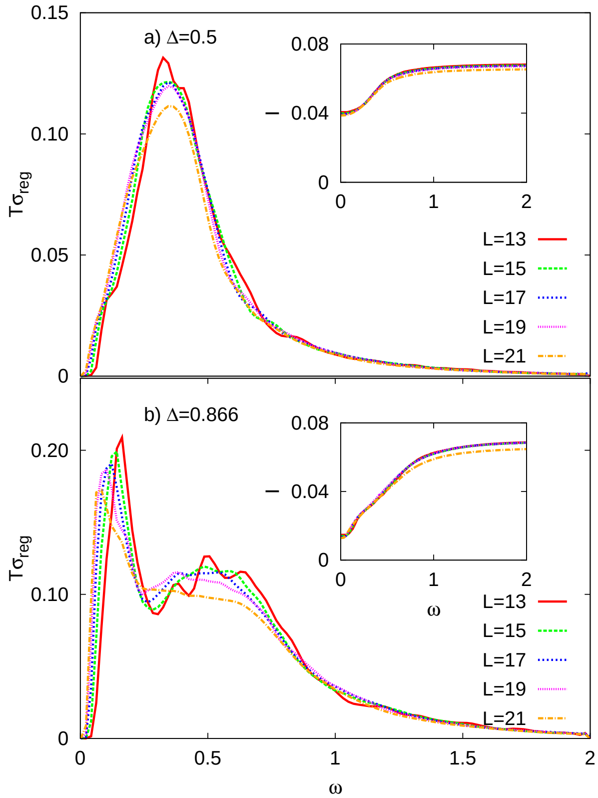

Figure 2. (Color online) Regular part of dynamical conductivity $\sigma_{reg}(\omega)$ and the integrated one $I(\omega)$ (inset) for $s = 0$ and: a) $\Delta = 0.5$, and b) $\Delta = 0.86$ for different sizes $L = 13 - 21$.

and fixed N,

$$e_{kin} = \beta \frac{J^2}{4} \frac{N}{L} \Big(1 - \frac{N-1}{L-1} \Big) \qquad (9)$$

In Fig. 2 we present characteristic results for $\sigma_{reg}(\omega)$ as well as $I(\omega)$ (in inset) for two commensurate values $\nu = 3, 6$, i.e., $\Delta = 0.5, \sqrt{3}/2 = 0.866$, respectively. We note that for $\Delta = 0.5$ the incoherent part in $\sigma_{reg}(\omega)$ is quite L-independent in a broad range $L = 13 - 21$ and consequently the convergence of obtained Drude weight C vs. $1/L$ is very stable. Less obvious case is $\Delta = 0.866$ ($\nu = 6$) being already closer to the critical value $\Delta = 1$. The incoherent $\sigma_{reg}(\omega)$ reveals here a low-ω contribution whereby the peak is shifting as with $1/L$ as observed even more pronounced for $\Delta > 1$ [16]. However, in the present case the peak intensity as well diminishes with L (a closer inspection reveals that the peak ω_p also vanishes here faster than $1/L$) so that the integrated $I(\omega)$ in Fig. 2b appears to have well defined limit $C = I(\omega \to 0)$.

In Fig. 3 we present $I(\omega)$ for $\Delta = 0.25$ characteristic for the regime $\Delta < 0.5$. We note that the high-ω part is quite L-independent (note that for L=21 we calculate only one k-vector, which influences slightly the sum rule $I(\omega \to \infty)$) similar to results for $\Delta = 0.5$ in Fig. 2a. However, there is also a well visible anomalous low-ω contribution at $0.02 < \omega < 0.08$ (see the inset). The peak in $\sigma(\omega)$ (as

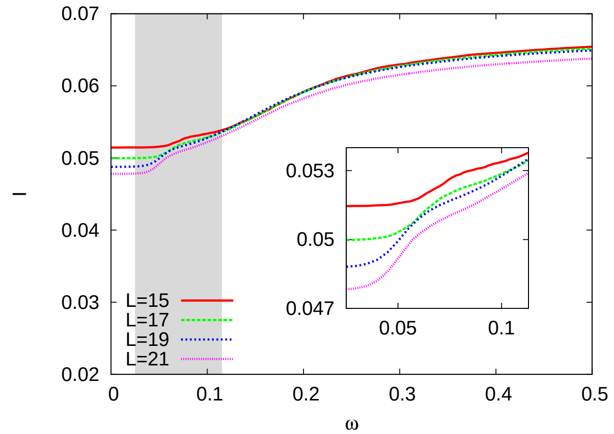

Figure 3. (Color online) Integrated dynamical conductivity $I(\omega)$ for $\Delta = 0.25, s = 0$ and various sizes L. The inset focuses on the low-ω regime.

obtained from $I(\omega)$ in the inset of Fig. 3) appears to shift towards $\omega_p = 0$ somewhat faster than $1/L$ (approximate fit $\omega_p \sim 1.342/L - 0.017$) whereas its weight in $I(\omega)$ increases with the system size. This deviation can be counted as an additional contribution to effective δC. This is, e.g., in contrast to case $\Delta = 0.866$, where the intensity decreases with L (Fig. 2). Although the origin of the low-ω anomaly is not well understood it seems that it is absent for commensurate values of $\Delta = \cos(\pi/\nu)$ which possess additional degeneracies [13].

Results for C vs. $1/L$ as in Fig. 1 can be used to extrapolated to the thermodynamic value C where we use the extrapolation $C(L) = C + \alpha/L + \zeta/L^2$. Obtained results for $C(\Delta)$ are presented in Fig. 4. On the other hand, one can correct $C(L)$with the low-ω contribution $\tilde{C}(L) = C(L) + \delta C(L)$ and get modified extrapolation $\tilde{C}$, also presented in Fig. 4. We can now compare the results with the analytical result obtained via Thermodynamic Bethe Ansatz (TBA) [13, 15],

$$C = \frac{\gamma - \frac{1}{2}\sin(2\gamma)}{16\gamma}, \quad \Delta = \cos(\gamma), \qquad (10)$$

the validity of which has been still questioned [12, 15]. We note that the agreement of the analytical form (10) with the corrected numerical $\tilde{C}$ is very satisfactory for $s = 0$ within the whole regime of Δ.

Let us now turn to the dependence of C on magnetization s (filling n). It is evident that one gets $C = 0$ within the Ising-type regime $\Delta > 1$ only for $s = 0$. Results for C at $\Delta = 1.7$ and $\Delta = 3$ are shown in Fig. 5 for fixed $L = 19$ and all available S_z. It is indicative that $C(s)$ are nearly equal for both $\Delta > 1$. To go beyond the finite-size results one can also perform the scaling to $L \to \infty$ analogous to $n = 1/2$ case which is possible, e.g., for $s = 1/4$ (taking into account results for $L = 5 - 25$) and $s = 1/3$ (with results for $L = 9 - 21$). Corresponding results for the extrapolated C are also plotted in Fig. 5, confirming that $C(s)$ become essentially universal

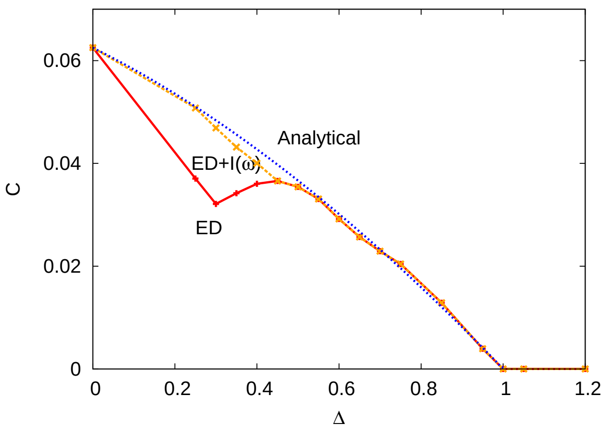

Figure 4. (Color online) High-T Drude weight $C = TD$ vs. Δ at magnetization $s = 0$ obtained: using the ED and finite-size scaling of $D(L)$ (full curve), adding the low-ω correction (dashed curve), and within the analytical TBA [13, 15] (dotted curve).

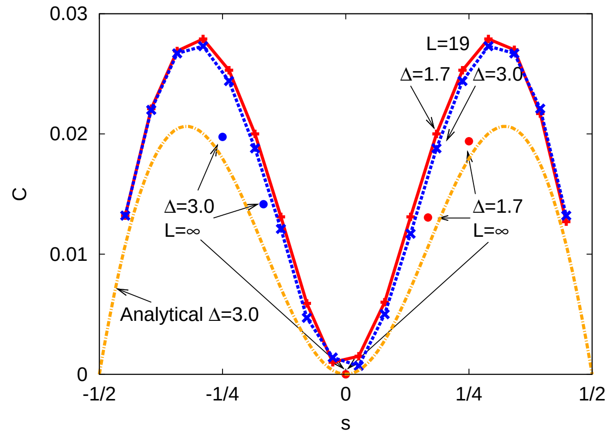

Figure 5. (Color online) High-T Drude weight C vs. magnetization s within the Ising-type regime $\Delta = 1.7, 3.$ obtained for fixed $L = 19$, with the $1/L \to 0$ extrapolation for $s = 0, 1/4, 1/3$ (dots), and the analytical approximation C_3, Eq.(11), for $\Delta = 3$.

for $\Delta > 1$.

It has been already observed in Ref.[5] that within the Ising regime $\Delta > 1$ the Drude weight can be via the Mazur inequality well exhausted with the overlap onto the simplest nontrivial local conserved quantity $Q_3 = j_E$ representing the energy current. At $T \to \infty$ this overlap can be evaluated exactly leading to

$$C_3 = \frac{1}{2L}\frac{\langle JQ_3\rangle^2}{\langle Q_3^2\rangle} = \frac{\Delta^2 s^2(1-4s^2)}{1+2\Delta^2(1+4s^2)}. \qquad (11)$$

From Fig. 5 we see that the agreement between the approximate C_3, Eq.(11), and the extrapolated C is nearly perfect for large $\Delta \gg 1$, e.g., $\Delta = 3$, while for $\Delta = 1.7$ the value C_3 starts to decrease, so that $C_3 < C$. In fact we observe from Eq.(11) that C_3 just saturates as a function of Δ for $\Delta \gtrsim 1.7 - 2$ and its value there can already reasonably reproduce C. We stress again completely different behavior is for $\Delta < 1$ and $s = 0$. In this case one gets $C_3 = 0$ (as well as higher overlaps $C_{n>3} = 0$ due to particle-hole symmetry), hence the Mazur inequality with local conserved quantities is unable to reproduce $C > 0$ at $s = 0$ [5].

Let us further consider the normalized Drude weight $D^* = D/e_{kin}$ which represents the relative weight of the dissipationless transport within the whole sum rule, Eq.(8), i.e., we have $0 < D^* < 1$. Since one cannot perform a systematic extrapolation $L \to \infty$ for arbitrary magnetization s we present in Fig. 6 results for D^* within the whole (half) plane $\Delta, s \geq 0$ as calculated in systems with fixed $L = 19$. Apart from some anomalies observed (without the correction δC) already in Fig. 3 we confirm quite regular dependence D^* on (Δ, s). It is quite evident that in the limiting case $\Delta = 0$ (XY model) we get $D^* = 1$ corresponding to noninteracting fermions where the whole sum rule is within the Drude weight. The same hold for maximal magnetization $s \to \pm 1/2$ (for nearly empty or full band, $n \to 0, n \to 1$, respectively)

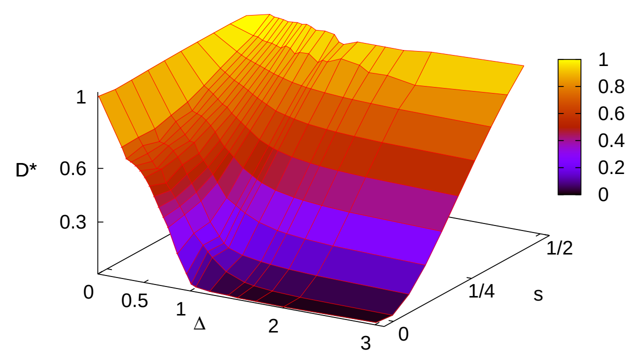

Figure 6. (Color online) Normalized Drude weight D^* within the plane Δ, s as calculated in systems with fixed size $L = 19$.

where the interaction does not play a role. For fixed Δ the minimum of D^* is always at $s = 0$ whereby the dependence $D^*(s)$ is nearly universal for all $\Delta > 1$.

B. Finite Temperature

Finally, let us present results for the T-dependence $D(T)$ as evaluated using the relation (6), again restricting our analysis to zero magnetization $s = 0$ and systems with odd L (Fig. 7). It should be realized that numerical results at low $T < 0.5$ are more susceptible to finite-size effects since very small number of MB levels effectively participate in $D(T)$ and the crucial contribution comes from the ground state $\epsilon_0(\phi)$. Still, in spite of some discrepancies at low $T < 0.4$ the overall agreement with the TBA result [13] is reasonable. Another conclusion is that the extended high-T behavior, i.e. $D = C/T$ is followed very accurately down to quite low $T > 0.5$ in the whole range

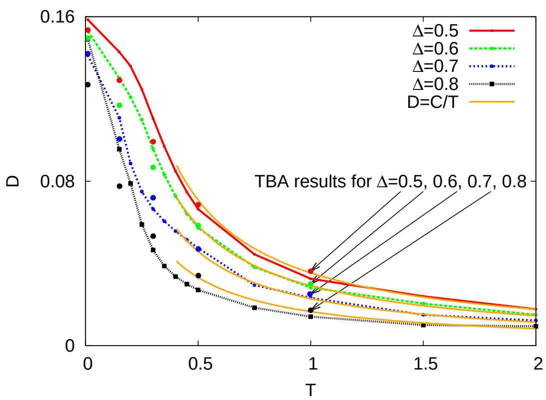

Figure 7. (Color online) Finite-T Drude weight $D(T)$ for $\Delta < 1$ at magnetization $s = 0$ as calculated numerically using ED with $L = 15 - 21$ and finite-size scaling (full line with dots), extrapolating the high-T numerical result, i.e. $D = C/T$ (thin lines), and Thermodynamic Bethe Ansatz result (dots) from Ref.[13].

$\Delta < 1$. While the ground state value D_0 is quite reliable in the intermediate window $0 < T < 0.5$ results are sensitive to finite-size effects so we cannot give a firm conclusion on possible nonanalytical low-T behavior as predicted in Ref.[13].

IV. CONCLUSIONS

In conclusion, we have shown that numerical evaluation of the Drude weight (spin stiffness) $D(T)$ within the anisotropic Heisenberg model can lead to more controlled and converged results if performed in a canonical ensemble, at fixed S_z (number of particles N). Breaking of the particle-hole symmetry by using systems with odd L is also helpful and is advantageous over usually studied systems with even L. Our study is mostly concentrated on the high-T limit which should be anyhow quite generic for the whole regime $T > 0$. Results obtained at zero magnetization $s = 0$ using the finite-size scaling confirm the change of character of $D(T)$ at $\Delta = 1$, i.e., they are compatible with the $D(T) = 0$ for $\Delta > 1$. While at $s = 0$ within the majority of the regime $\Delta < 1$ there are no evident problems with the scaling $1/L$ of $D(T)$ we have traced the irregularities at $\Delta < 0.5$ back to the emergence of finite-size low-ω contribution in $\sigma_{reg}(\omega)$ which can lead to a finite correction δC in the thermodynamic limit $L \to \infty$. Taken the latter into account, we find a very good agreement with the TBA result [13], in this way possibly eliminating (or at least restricting) some recently expressed questions regarding its validity.

High-T normalized Drude weight D^* away from $s = 0$ shows a systematic and smooth variation with s towards the limiting values $D^* = 1$ for $s = \pm 1/2$ as well as in XY limit $\Delta = 0$. In the Ising regime $\Delta > 1$ (in particular for large $\Delta > 2$) the variation $C = TD(s)$ is very well reproduced with the Mazur inequality overlap with the conserved energy current j_E, in very contrast to the XY-type regime $\Delta < 1$.

Results for the T-variation $D(T)$ reveals that even quantitatively the high-T result $D = C/T$ remains valid in a wide regime, i.e., generally for $T > 0.5$. While small-system results allow also for a reliable scaling for $D_0 = D(T = 0)$ at $s = 0$, the finite-size effects are rather hard to avoid in the window $0 < T < 0.5$ and other methods beyond the ED are needed to investigate in more detail this regime.

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[1] for a review, see X. Zotos and P. Prelovšek, in *Strong Interactions in Low Dimensions*, eds. D. Baeriswyl and L. Degiorgi (Kluwer Academic Publishers), p. 347-382 (2004)
[2] for a review, see F. Heidrich-Meisner, A. Honecker and W. Brenig, Eur. Phys. J. Special Topics **151**, 135 (2007).
[3] H. Castella, X. Zotos and P. Prelovšek, Phys. Rev. Lett. **74**, 972 (1995).
[4] B. S. Shastry, B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990).
[5] X. Zotos, F. Naef and P. Prelovšek, Phys. Rev. B **55**, 11029 (1997).
[6] M. S. Hawking, M. Long and X. Zotos, arXiv:cond-mat/0812.3096 (unpublished).
[7] T. Prosen, Phys. Rev. Lett. **106**, 217206 (2011).
[8] X. Zotos and P. Prelovšek, Phys. Rev. B **53**, 983 (1996).
[9] B. N. Narozhny, A. J. Millis and N. Andrei, Phys. Rev. B **58**, R2921 (1998).
[10] F. Heidrich-Meisner, A. Honecker, D. C. Cabra and W. Brenig, Phys. Rev. B **68**, 134436 (2003).
[11] M. Rigol and B. S. Shastry, Phys. Rev. B **77**, 161101(R) (2008).
[12] J. Sirker, R. G. Pereira and I. Affleck, Phys. Rev. Lett. **103**, 216602 (2009).
[13] X. Zotos, Phys. Rev. Lett. **82**, 1764 (1999).
[14] W. Kohn, Phys. Rev. **133**, A171 (1964).
[15] J. Benz, T. Fukui, A. Klümper and C. Scheeren, J. Phys. Soc. Jpn. Supp. **74**, 181 (2005).
[16] P. Prelovšek, S. El Shawish, X. Zotos and M. Long, Phys. Rev. B **70**, 205129 (2004).